Commutator-errors in large-eddy simulation

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Abstract

A new formulation is derived for the commutator-errors in large-eddy simulation of incompressible flow. These commutator-errors arise from the application of non-uniform filters to the Navier-Stokes equations. As a consequence, the filtered velocity field is no longer solenoidal. The order of magnitude of the commutator-errors is compared with the divergence of the turbulent stresses. This shows that one can not reduce the size of the commutator-errors independently of the turbulent stress terms by some judicious construction of the filter operator. Similarity modeling for the commutator-errors is presented, including an extension of Bardina's approach and the application of Leray regularization. The performance of the commutator-error parameterization is illustrated with the one-dimensional Burgers equation. For large filter-width variations the Leray approach is shown to capture the filtered flow with better accuracy than is possible with Bardina's approach.

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The desire to extend large-eddy simulation (LES) to complex flows generally implies that one is confronted with strongly varying turbulence intensities within the flow-domain and also as a function of time. In certain regions of the flow a nearly laminar flow may arise while a lively, fine-scale turbulent flow can be present simultaneously in another region. In the filtering approach this can be accommodated using a filter operator with non-uniform filter-width that may depend on both space and time. The use of such filters, however, further complicates the subgrid closure problem through the appearance of additional commutator-errors [1]. We will formulate a systematic modeling of the dynamics of these contributions.

Distinguishing between which flow-features are 'subgrid' and which are 'resolved', depends on the local filter-width Δ. Spatial and temporal variations in Δ therefore imply additional energy transfer mechanisms among the scales in the flow, besides the well-known energy-transfer due to the quadratic nonlinearity in the Navier-Stokes equations. If a flow structure propagates from a region of small filter-width into a region with strongly increased filter-width, it would appear as if part of this structure would turn from a 'resolved' to a 'subgrid' feature, merely by translation. The reverse can also be imagined, leading to the apparent emergence of resolved structures from a collection of subgrid scales. This suggests additional sources of local energy drain or backscatter, depending on the specific local filter-width variations in the direction of the instantaneous local flow which require explicit parameterization.

The traditional use of convolution filters in LES necessarily implies that the width of the filter is constant. However, efficient extension of the LES approach to turbulent flows in complex geometries or to cases with strong spatial variation of turbulence intensities, calls for the introduction of non-uniform filter-widths. The starting point is an extended filter L which, in one spatial dimension, is defined by

$$\overline{u}(x,t) = L(u)(x,t) = \int_{x-\Delta_-(x,t)}^{x+\Delta_+(x,t)} \frac{H(x,\xi)}{\Delta(x,t)} u(\xi,t) \, d\xi \tag{1}$$

where $\Delta_\pm$ denote the upper and lower bounds and $\Delta = \Delta_+ + \Delta_-$. In complex flow geometries the variations in turbulence intensities poses different local requirements on the amount of

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detail with which the flow should be represented. Such a situation can be formulated by allowing a non-uniform filter-width as given in (1). The application of such filters gives rise to a number of extra closure terms in addition to the well-known turbulent stresses.

If one applies the filter (1) to the incompressible flow equations, commutator-errors arise since $\overline{\partial_x u} \neq \partial_x \overline{u}$ or, written differently, $L(\partial_x u) - \partial_x(L(u)) = [L, \partial_x](u) \neq 0$ in terms of the commutator of L and the derivative operator ∂_x. For the filtered continuity equation we find

$$\partial_j \overline{u}_j = -[L, \partial_j](u_j) \tag{2}$$

Hence, the filtered continuity equation is no longer in local conservation form and variations in the filter-width imply that $\overline{u}_j$ is not solenoidal. Filtering the Navier-Stokes equations in the same way yields

$$\begin{aligned}
\partial_t \overline{u}_i + \partial_j(\overline{u}_i \overline{u}_j) + \partial_i \overline{p} - \frac{1}{Re} \partial_{jj} \overline{u}_i = -\Big(& [L, \partial_t](u_i) \\
& + \partial_j([L, S](u_i, u_j)) + [L, \partial_j](S(u_i, u_j)) \\
& + [L, \partial_i](p) - \frac{1}{Re}[L, \partial_{jj}](u_i) \Big)
\end{aligned} \tag{3}$$

We observe that commutators emerge of filtering and the product operator $S(f, g) = fg$ as well as commutators of filtering and first and second order partial derivatives. Filtering a linear term such as $\partial_t u_i$ gives rise to a 'mean-flow' term $\partial_t \overline{u}_i$ and a corresponding commutator-error $[L, \partial_t](u_i)$. Filtering the nonlinear convective terms leads to the divergence of the turbulent stress tensor $\tau_{ij} = \overline{\overline{u}_i \overline{u}_j} - \overline{u}_i \overline{u}_j = [L, S](u_i, u_j)$ and an associated commutator-error $[L, \partial_j](S(u_i, u_j))$. The local conservation form of the Navier-Stokes equations is no longer maintained, in the same way as observed in (2).

The commutators in (2) and (3) satisfy algebraic identities. If we consider any two filters L_1 and L_2 then

$$[L_1 L_2, S] = [L_1, S]L_2 + L_1[L_2, S] \tag{4}$$

which is known as Germano's identity [2]. Likewise,

$$[L_1, [L_2, S]] + [L_2, [S, L_1]] + [S, [L_1, L_2]] = 0 \tag{5}$$

which is interpreted as Jacobi's identity. These identities are also satisfied by $[L, \partial_t]$ and $[L, \partial_j]$ which shows that the structure of the LES closure problem is closely related to the Poisson-bracket in classical mechanics. In that context Germano's identity is known as Leibniz' rule. The identities (4) and (5) can be used to guide (dynamic) subgrid modeling of the central commutators.

Filtering the incompressible flow equations gives rise to an 'LES-template' in which the 'Navier-Stokes' operator on the left hand side of (3) acts on the filtered solution $\{\overline{u}_i, \overline{p}\}$. In addition, a number of unclosed terms arises of which only the parameterization of the turbulent stresses attracted considerable attention in literature. However, the subgrid modeling problem associated with non-convolution filters entails various additional commutator-errors. These terms require explicit modeling in case the spatial and temporal variations of the filter-width are sufficiently large. For steady filter-width distributions, to which we restrict ourselves here, the magnitude of these contributions can be quantified in terms of $\overline{\mathbf{u}} \cdot \nabla \Delta = \overline{u}_j \partial_j \Delta$.

The dynamic effects of the commutator-errors have been considered unimportant by some authors, provided a suitable class of filters would be adopted. In [3] such a class of filters was constructed and the commutator-errors corresponding to these filters could be made of high order in Δ. Likewise, [4] considers the commutator-errors to be of minor importance in case high order filters are used. Although it is correct that the commutator-errors can be made small with the proper filter, one has to realize that with the same filter the divergence of the turbulent stress tensor is also reduced to the same order in Δ. The use of higher order filters would hence only imply a gradual convergence to the unfiltered Navier-Stokes equations. It is not possible to reduce the size of the commutator-errors *independently* of $\partial_j([L, S](u_i, u_j))$ merely by constructing suitable filters. The subgrid modeling of the dynamic significance of the commutator-errors therefore remains a largely open problem.

In order to establish the importance of the commutator-errors relative to the turbulent

stress contributions we introduce general N-th order filters by requiring $L(x^m) = x^m$ for $m = 0, 1, \ldots, N - 1$ [4]. Application of such a filter yields:

$$\overline{u}(x) - u(x) = \sum_{m \geq N} \left(\Delta^m(x) M_m(x) \right) u^{(m)}(x)$$

where $u^{(m)}$ denotes the m-th derivative and $M_m(x)$ is related to the m-th moment of L. To leading order $\overline{u} - u \sim \Delta^N$. For the commutator-error we find

$$[L, \partial_x](u) = - \sum_{m \geq N} \left(\Delta^m M_m \right)' u^{(m)}$$

where the prime denotes differentiation with respect to x. The commutator $[L, S](u)$ can be expressed as:

$$[L, S](u) = \sum_{m \geq N} \left(\Delta^m M_m \right) \left((u^2)^{(m)} - 2uu^{(m)} \right) - (\overline{u} - u)^2$$

The scaling of the turbulent stresses with Δ^N is readily verified for $N > 1$. In case $N = 1$ the commutator scales with Δ^2 since $(u^2)' = 2uu'$. Combining these expressions one may obtain the leading order behavior of the flux terms for symmetric filters as:

$$[L, \partial_x](S(u)) \approx A(x) \left(\Delta^{N-1} \Delta' M_N \right) + B(x) \left(\Delta^N M_N' \right)$$
$$\partial_x([L, S](u)) \approx a(x) \left(\Delta^{N-1} \Delta' M_N \right) + b(x) \left(\Delta^N M_N' \right)$$
$$+ c(x) \left(\Delta^N M_N \right) \tag{6}$$

where A, B, a, b and c are smooth, bounded functions which contain combinations of derivatives of the solution u. For non-uniform filters $[L, \partial_x](S) \sim \Delta' \Delta^{N-1}$ which is the same leading order behavior as for $\partial_x[L, S]$. Hence, it is not possible to remove only the commutators $[L, \partial_x]$ by a careful construction of the filter [3]. In fact, all filters that would reduce $[L, \partial_x]$ are of higher order and consequently will also reduce $[L, S]$ with the same order.

One may use a Fourier-mode analysis to relate the dynamic significance of the commutator-errors to variations in Δ and the wavenumber k of the mode. For second order filters such as the top-hat or Gaussian filter one has

$$\frac{\|[L, \partial_x](S(u))\|}{\|\partial_x([L, S](u))\|} \sim \frac{|\Delta'/\Delta|}{|k|} \tag{7}$$

where $\| \cdot \|$ denotes the L_2-norm. This shows that if $|\Delta'| \ll |k\Delta|$ then filter-width non-uniformity can be disregarded and it should be sufficient to model only τ_{ij}. This shows that only strongly bounded variations in the filter-width will reduce the size of the commutator-errors significantly while keeping the magnitude of the turbulent stresses unaffected. If, however, for efficiency reasons or due to, e.g., wall-proximity, a sufficiently smooth variation of Δ is not possible, one has to resort to direct modeling of the commutator-errors.

In the absence of a comprehensive theory of turbulence and its non-uniform spatial and temporal representations, the modeling of the turbulent stresses and the commutator-errors relies to some degree on limited empirical knowledge. Here we restrict ourselves to similarity modeling and consider two different approaches. Specifically, we will extend Bardina's approach [5] to include commutator-errors and we derive the implied subgrid models arising from Leray regularization [6].

Bardina's similarity model for the turbulent stress tensor arises from applying the definition of τ_{ij} to $\overline{u}_i$, i.e.,

$$\tau_{ij} \rightarrow m_{ij}^B = [L, S](\overline{u}_i, \overline{u}_j) = \overline{\overline{u}_i \overline{u}_j} - \overline{\overline{u}}_i \overline{\overline{u}}_j \tag{8}$$

Extending this idea to the commutator-error suggests the following parameterization: $[L, \partial_j](u_i u_j) \rightarrow [L, \partial_j](\overline{u}_i \overline{u}_j)$. In [7] this model showed a high correlation for turbulent boundary layer flow which partially substantiates this approach.

Recently, the Leray regularization principle [6] was revived in the context of LES [8]. In this approach the convective fluxes are replaced by $\overline{u}_j \partial_j u_i$, i.e., the solution $\mathbf{u}$ is convected with a smoothed velocity $\overline{\mathbf{u}}$. The governing Leray equations can be written as [6]

$$\partial_j u_j = 0 \quad ; \quad \partial_t u_i + \overline{u}_j \partial_j u_i + \partial_i p - \frac{1}{Re} \partial_{jj} u_i = 0 \tag{9}$$

This formulation can be written in terms of $\{\overline{u}_i, \overline{p}\}$ in case we assume a (formal) inverse L^{-1} of L, i.e., $u_j = L^{-1}(\overline{u}_j)$. After some calculation one obtains the filtered continuity equation (2) and the filtered momentum equation as

$$\partial_t \overline{u}_i + \partial_j(\overline{u}_i \overline{u}_j) + \partial_i \overline{p} - \frac{1}{Re} \partial_{jj} \overline{u}_i = -\Big([L, \partial_t](u_i)$$
$$+ \Big\{ \partial_j(m_{ij}^L) + \overline{u_i \partial_j \overline{u}_j} \Big\} + [L, \partial_j](S(u_i, \overline{u}_j))$$
$$+ [L, \partial_i](p) - \frac{1}{Re}[L, \partial_{jj}](u_i)\Big) \tag{10}$$

The divergence of the turbulent stress tensor in (3) is represented in terms of the asymmetric, filtered similarity-type Leray model m_{ij}^L and an additional term associated with the divergence of the filtered velocity field:

$$\partial_j \tau_{ij} \rightarrow \partial_{ij}(m_{ij}^L) + \overline{u_i \partial_j \overline{u}_j} \tag{11}$$

where $m_{ij}^L = \overline{\overline{u}_j u_i} - \overline{u}_j \overline{u}_i$ [8] and the commutator-error is expressed as $[L, \partial_j](u_i u_j) \rightarrow [L, \partial_j](\overline{u}_j u_i)$. The other commutator-errors are identical to those in (3) with the understanding that in actual simulations every occurrence of an unfiltered flow-variable implies the application of L^{-1} to the available field. The Leray model was shown to provide good predictions of three-dimensional turbulent mixing at arbitrarily high Reynolds number using a uniform filter [8].

To assess the effects of the commutator-errors and determine the quality of the Bardina and Leray modeling we consider the one-dimensional Burgers equation. This provides a model-system which has the same basic structure under filtering as expressed in (3). All relevant commutators appear in the filtered Burgers equation. The initial solution is a Gaussian profile which rapidly develops into the well-known 'ramp-cliff' structure. We use $Re = 500$ to obtain a sharply localized cliff region, and apply periodic boundary conditions. Explicit time-integration, restricted by stability time-steps, and second order accurate spatial discretization are adopted. To avoid numerical errors we use high spatial resolution, typically with $N = 2048$ intervals. Explicit filtering is done with trapezoidal quadrature applied to the top-hat filter.

We consider a non-uniform grid with grid-spacing $h_i = (\ell/N)(1 + g_i)$ where ℓ is the length of the domain. The grid is chosen to be non-uniform only in an interval around $i = N/2$ in computational space. For the illustrations we use

$$g_i = A \sin \left(2\pi \frac{(i - N/2)}{(N(m - 2q)/m)}\right) \quad ; \quad \frac{qN}{m} \leq i \leq \frac{(m - q)N}{m}$$

and 0 otherwise. Since $\sum g_i = 0$ this grid preserves the end-points. The parameters q and m control the region where the grid is non-uniform. Here, we use $q = 3$ and $m = 8$. The local filter-width $\Delta_i = x_{i+n} - x_{i-n}$ where n is chosen such that $\Delta = \ell/D$ with $D = 8$ or 16 in the uniform regions of the grid. With $N = 2048$ this implies $n = 128$ or 64 respectively. The parameter $A < 1$ controls the ratio between largest and smallest intervals $(1 + A)/(1 - A)$.

In figure 1 we collected the contributions to the total convective flux for a representative uniform and non-uniform case. We decomposed the convective flux as

$$\overline{\partial_x(u^2)} = \partial_x(\overline{u}^2) + \partial_x(\overline{u^2} - \overline{u}^2) + \{\overline{\partial_x(u^2)} - \partial_x(\overline{u^2})\}$$

identifying on the right hand side the 'mean' flux, the 'SGS-flux' and the 'commutator-flux' respectively. In figure 1 the solution and the filtered solution are included displaying the 'ramp-cliff' structure. The total flux in figure 1(a) is piecewise linear and the SGS flux is localized in the cliff-region where filtering is effective. In figure 1(b) there is a significant distortion of the filtered solution due to the filter-width non-uniformity. Two characteristic contributions due to the commutator-error arise. On the 'ramp side', the non-uniform filter-width near $x = -3$ strongly influences the mean flux. The commutator-error compensates for this such that the total flux remains nearly linear in x. Within the 'cliff-region' the commutator-flux is comparable to the SGS-flux.

In figure 2(a) we show the locations of the front and back of the ramp-cliff solution as a function of time. These locations are defined where $|u|$ equals $\varepsilon \max(|u|)$ with $\varepsilon = 0.05$. Comparing filtered Burgers results with predictions from the Leray and Bardina parameterizations, the Leray results are more accurate. This was confirmed by considering the minimal and maximal values of u which are also better predicted by the Leray model. The L_2-norm of the fluxes for these cases show that the commutator-flux is about 1/3-1/2 the value of the SGS-flux. In cases with smaller grid non-uniformities the direct Leray modeling still enhances the accuracy of the predictions notably. The Leray model is considerably less

expensive than the Bardina model and it also better preserves qualitative properties of the filtered Burgers solution cf. figure 2(b). The Bardina parameterization creates additional structure in the solution, which is not present in the filtered Burgers result.

The commutator-errors have been expressed as commutators of filtering and partial derivatives. The magnitude of the commutator-errors can not be reduced independently of the SGS-fluxes. Instead, for sufficiently large grid non-uniformities direct modeling is needed. For the one-dimensional Burgers equation the Leray parameterization combines computational efficiency with high accuracy. This motivates the use of the Leray commutator model in more complex flows. The a priori specification of the spatial filter-width variations is not generally possible for complex cases. Therefore, the local filter-width needs to be related to the resolved solution to facilitate a dynamic response of local filtering and the evolving flow. This is subject on ongoing research.

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FIG. 1. Snapshot of the solution (multiplied by 1/2) (solid) and filtered solution (solid; markers o). Convective flux: total (dots), mean (dash-dotted), turbulent stress (dashed), commutator-error (solid with $*$). In (a) we use $\Delta = \ell/16$ and in (b) the non-uniform case with $A = 1/2$ is shown. Underneath in (b), the grid-spacing (minus 0.2) as a function of x is presented.

FIG. 2. Location of the head of the cliff (upper curves) and the tail of the ramp (lower curves) in (a) and in (b) snapshot of the filtered solution: filtered Burgers (solid), Leray (dashed) and Bardina (dash-dotted) for $A = 0.85$
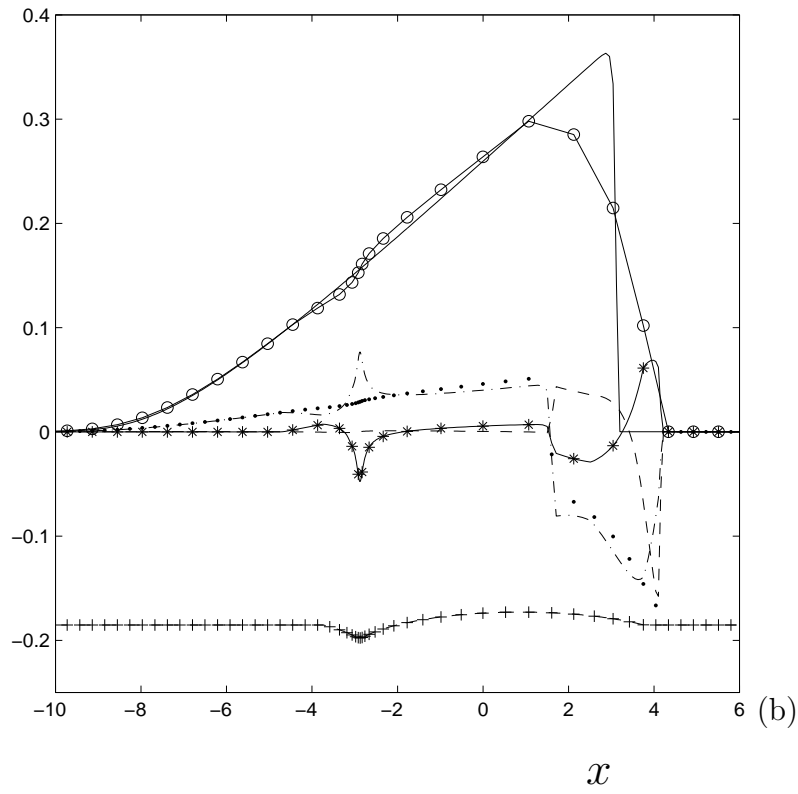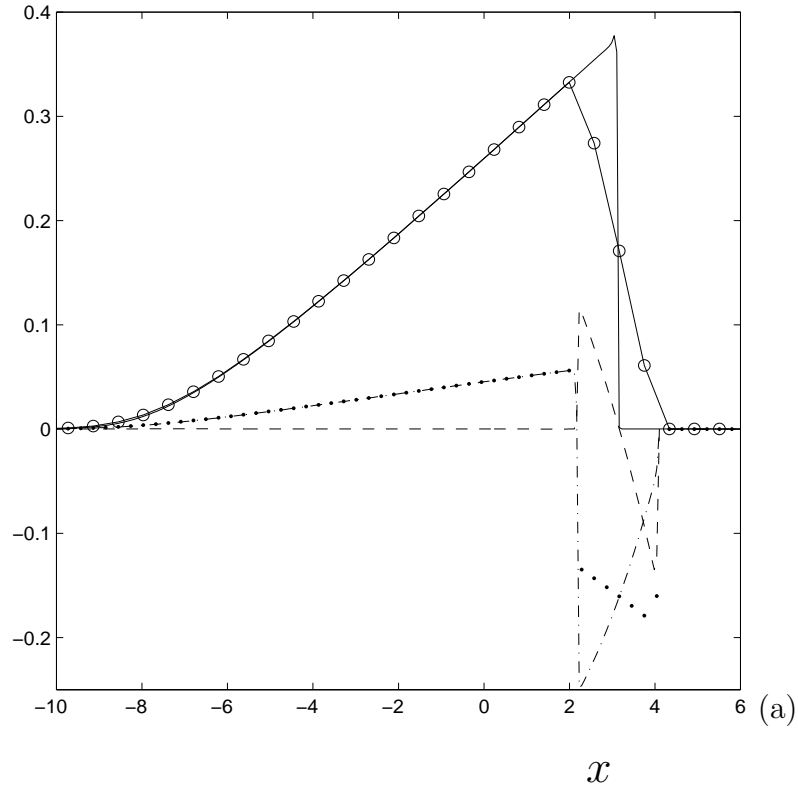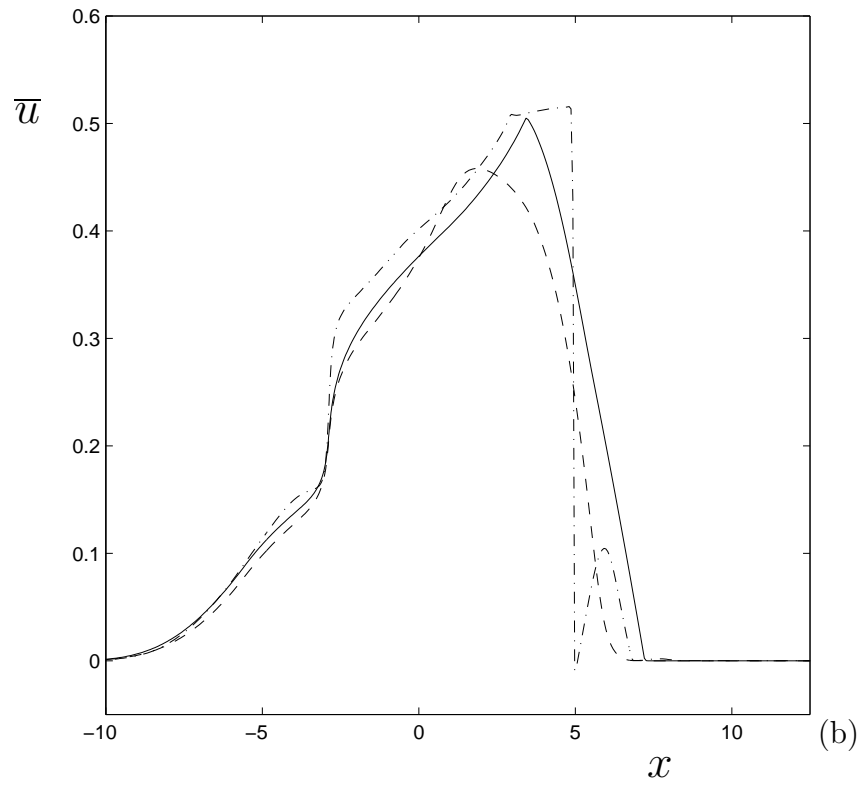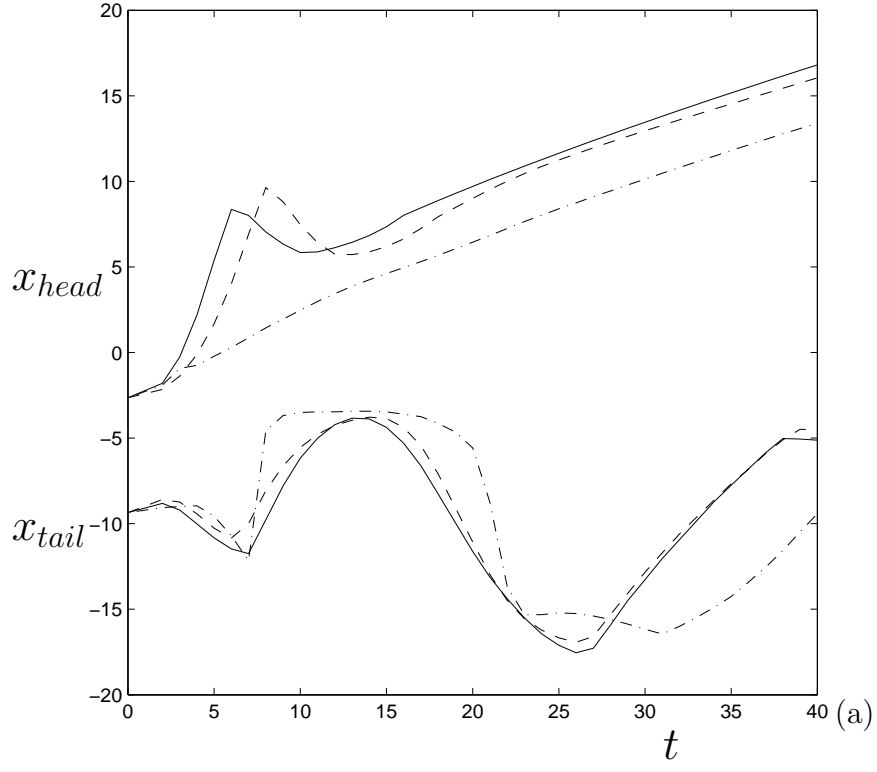
FIG. 1. Geurts, Holm: Phys.Fluids

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FIG. 2. Geurts, Holm: Phys.Fluids

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